Indian Journal of Pure & Applied Physics
Vol. 63, October 2025, pp. 961-967
DOI: 10.56042/ijpap.v63i10.21814

# Theoretical Modeling of Elastic, Thermal and Ultrasonic Properties of B1-Dysprosium Monopnictides

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*Received: 19th July 2025; accepted: 15th September*

Nonlinear elastic and thermoacoustical investigation of heavy rare earth pnictides DyPn (Pn=P, As, Sb, Bi) has been carried out at different temperature in different directions. The second and third order, elastic constants for B1 structured DyPn have been obtained in temperature interval 0-300K applying Born-Mayer potential model. The Cauchy and Born stability criteria predict that DyPn are elastically stable. The bulk and shear modulus are decreasing with atomic number which is highest for DyP and lowest for DyBi. The shear modulus to bulk modulus ratio are less than 0.57 which illustrates that chosen DyPn are brittle in temperature span 0-300K. The ultrasonic characteristics of DyPn have been tudied by calculating ultrasonic velocities, thermal conductivity, relaxation time and Grüneisen parameter. The Debye characteristic temperature and thermal conductivity are highest for DyP at 100K along <111> direction for best suited thermal performance. The results of thermal relaxation time show that chosen DyPn are semimetallic in nature. The nonlinear Gruneisen parameter increases as DyBi>DySb>DyAs>DyP. The results in present study are calculated precisely and compared with previous structured values.

**Keywords:** Elastic constant, Mechanical properties, Debye temperature, Thermal conductivity, Grüneisen parameter

## 1 Introduction

Due to significance structural, electronic and magnetic properties the heavy rare earth chalcogenides and pnictides owe great attention among researchers. The lattice structure and elastic moduli for B1 structured DyP and DyAs have been studied by Özısık *et al*.[1] in which they have reported the bulk modulus, Zener anisotropy, Young modulus and Debye temperature using ab-initio method. Effect of high pressure on elastic, structural and thermal behaviour of DyP and DyAs has been examined by Bhajanker *et al*.[2] using inter ionic potential model to predict the magnitudes of second order elastic constants, Poisson ratio, other elastic moduli and cohesive energy. The magnetic properties of DySb with respect to temperature in 23.6 kOe have been expressed by Everett *et al*.[3] and prepared base for magnetic characteristics of dysprosium pnictides. Gupta *et al*.[4] have calculated the elastic constants, modulus of elasticity and structural parameters of DySb based on first principle approximation. The study predicts that DySb is semimetallic. The magnetic properties of DyBi has been examined by Hulliger[5] at 52 kOe and found magnetic ordering in DyBi. The shear elastic constant for DySb near the magnetic and structural phase transition has been studied by Moran *et al*.[6] and Ray *et al*.[7] and these studies found that above 9.5 K there is phase transition and shear modulus does not continue to be softening also found that cubic structure changes to tetragonal. The magnetoelastic constants of DySb have been calculated by Morin *et al*.[8]. The optical properties of DyP and DyBi single crystal have been measured by Schoenes *et al*.[9] on the basis of local density approximation between 0.03 and 12eV. The electronic and optical properties of dysprosium pnictides have been examined by Schoenes et al.[10] in further studies in which they have reported that dysprosium pnictides are poor metals. The lattice structure of NaCl type single crystal DyBi has been examined by Zhao *et al*.[11] and value of lattice parameter has been calculated by them. Various literatures of B1/B2 structured pnictides of different materials like fermium monopnictides[12], curium monopnictides[13], boron monopnictides[14], lanthanum monopnictides[15] and neptunium monopnictides[16] are available which cover elastic, thermal, mechanical and ultrasonic properties of pnictides.

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But there is no literature available covering the thermoelastic and ultrasonic properties of dysprosium pnictides. This prompted us to investigate DyPn (Pn: P, As, Sb, Bi) in NaCl-type rock salt structure to explore its elastic, mechanical and ultrasonic properties in the temperature range 100-300 K along <100>, <110> and <111> directions.

## 2 Theory

The n[th] order elastic constant in term of tensor notation can be expressed as[17]

$$C_{ijklmn} = \left( \frac{\partial^n F}{\partial \eta_{ij} \partial \eta_{ij} \partial \eta_{ij} \ldots} \right)_{\eta=0} \quad \ldots (1)$$

The Voigt notations replace tensor notations as[18]

$$C_{IJK} \ldots = C_{ijklmn} \ldots = \left( \frac{\partial^n F}{\partial \eta_{ij} \partial \eta_{ij} \partial \eta_{ij} \ldots} \right)_{\eta=0} \quad \ldots (2)$$

The indices *i,j,k* are modified as *ij=I*, *jk=J*, 11→1, 22→2, 33→3, 23→4, 31→5,12→6. The free energy *F* is expressed at temperature T as

$F=E+F^{vib}$ where

$$F^{vib} = F^{Vib} = \frac{k_B T}{n V_C} \sum_{i=0}^{3sN} \ln 2 \sinh(\hbar\omega_i / 2k_B T) \quad \ldots (3)$$

The symbols *E* is intrinsic energy, *VC* = unit cell volume, *n* = number of atoms, $K_B$ Boltzman Constants = number of ions

The energy *E* is expressed as

$$E = \frac{1}{2V_C} \sum \phi_{\mu\upsilon}(r) \quad \ldots (4)$$

$\phi_{\mu\upsilon}$(r) is the interaction potential between μ[th] and ν[th] ions which is sum of Coulomb potential $\phi_C(r)$ and Born-Mayer potential $\phi_{BM}(r)$.

$$\phi_C(r) = \pm \frac{e^2}{r}\,;\ \phi_{BM}(r) = Aexp\,(-\frac{r}{b}) \quad \ldots (5)$$

The second and third order elastic constant consists of two parts

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{Vib} \text{ and } C_{IJK} = C_{IJK}^0 + C_{IJK}^{Vib} \quad \ldots (6)$$

First part with superscript *0* is static elastic constant while second part with superscript "*vib*" expresses the vibrational contribution of elastic constant. The detailed formulae to calculate static and vibrational parts of elastic constants for NaCl type B1 structured DyPn are given in literature[19]. Mechanical behaviour of cubic crystals is determined by elastic moduli, Zener anisotropy index and Poisson ratio. The expressions for mechanical parameters are derived from our previous article[20]. When ultrasonic wave passes through crystalline material it is bifurcated in longitudinal ($V_L$) and shear modes ($V_{S1}$ and $V_{S2}$). The average of longitudinal and shear modes are used to define Debye velocity[21] as

$$\frac{3}{V_D^3} = \frac{1}{V_L^3} + \frac{1}{V_{S1}^3} + \frac{1}{V_{S2}^3} \quad \ldots (7)$$

The Debye temperature ($\theta_D$) an interlinking bridge between elastic and thermal properties are explored by Debye velocity as[20]

$$\theta_D = \frac{h}{k} \left[ \frac{3n}{4\pi} \left( \frac{N_a \rho}{M} \right) \right]^{1/3} V_D \quad \ldots (8)$$

where *n* is number of atoms, *k* Boltzmann constant, $\rho$ is density of material, $N_a$ is Avogadro's number and *M* is molar mass.

The Debye temperature is applied to calculate thermal conductivity from the formula given as[21]

$$\kappa = \frac{A\overline{M_a}\delta\theta_D^3\ n^{1/3}}{\gamma^2 T} \quad \ldots (9)$$

Thermal conductivity is further applied to calculate thermal relaxation time[21].

$$\tau_{th} = \tau_{Shear} = \frac{\tau_{Long}}{2} = \frac{3\kappa}{C_V V_D^2} \quad \ldots (10)$$

One of the very important thermal properties the ultrasonic Grüneisen parameter in tensor of the first order is expressed as[22]

$$\gamma_{\alpha\beta}^i = -\omega_i^{-1} \frac{\partial \omega_i(q)}{\partial \eta_{\alpha\beta}} \quad \ldots (11)$$

The average Grüneisen parameter and square average of Grüneisen parameter are explored by SOECs and TOECs along <100>, <110> and <111> directions[23].

## 3 Results and Discussion

The nearest neighbour distance $r_0$ for B1 structured DyP=2.83Å[2], DyAs=2.91Å[2], DySb=3.06Å[4] and DyBi=3.12Å[11] are chosen respectively while hardness constant is chosen 0.303[24] to find out second and third order elastic constants. The computed results of higher order elastic constants within 0-300K temperature range are arranged in Table 1.

The second order elastic constants (SOECs) are increasing in order DyP>DyAs>DySb>DyBi which establish an inverse relation between SOECs

Table 1 — Second and third order elastic constants ($10^{10}$N/m$^2$)

| Material | Temp(K) | $C_{11}$ | $C_{12}$ | $C_{44}$ | $C_{111}$ | $C_{112}$ | $C_{123}$ | $C_{144}$ | $C_{166}$ | $C_{456}$ | *Ref.* |
|---|---|---|---|---|---|---|---|---|---|---|---|
| DyP | 0 | 4.99 | 1.45 | 1.45 | -83.10 | -5.90 | 2.43 | 2.43 | -5.90 | 2.43 | |
| | | 16.73 | 4.06 | 4.09 | | | | | | | [2] |
| | 100 | 5.29 | 1.43 | 1.46 | -86.31 | -6.14 | 1.92 | 2.44 | -5.95 | 2.43 | |
| | 200 | 5.49 | 1.38 | 1.46 | -88.12 | -6.23 | 1.42 | 2.45 | -5.98 | 2.43 | |
| | 300 | 5.71 | 1.34 | 1.47 | -90.21 | -6.35 | 1.00 | 2.46 | -6.02 | 2.43 | |
| DyAs | 0 | 4.73 | 1.29 | 1.29 | -80.03 | -5.23 | 2.18 | 2.18 | -5.23 | 2.18 | |
| | | 15.02 | 3.58 | 3.60 | | | | | | | [2] |
| | 100 | 4.99 | 1.26 | 1.30 | -82.77 | -5.41 | 1.67 | 2.19 | -5.27 | 2.18 | |
| | 200 | 5.20 | 1.22 | 1.30 | -84.79 | -5.52 | 1.16 | 2.20 | -5.30 | 2.18 | |
| | 300 | 5.42 | 1.18 | 1.31 | -86.96 | -5.64 | 0.65 | 2.21 | -5.33 | 2.18 | |
| DySb | 0 | 4.27 | 1.04 | 1.04 | -74.36 | -4.17 | 1.79 | 1.79 | -4.17 | 1.79 | |
| | 100 | 4.51 | 1.00 | 1.04 | -76.94 | -4.33 | 1.27 | 1.79 | -4.20 | 1.79 | |
| | 200 | 4.71 | 1.00 | 1.04 | -79.03 | -4.44 | 0.76 | 1.80 | -4.22 | 1.79 | |
| | 300 | 4.92 | 0.93 | 1.05 | -81.22 | -4.56 | 0.25 | 1.81 | -4.25 | 1.79 | |
| DyBi | 0 | 4.11 | 0.96 | 0.96 | -72.34 | -3.84 | 1.66 | 1.66 | -3.84 | 1.66 | |
| | 100 | 4.33 | 0.93 | 0.96 | -74.84 | -4.00 | 1.15 | 1.67 | -3.87 | 1.66 | |
| | 200 | 4.54 | 0.89 | 0.97 | -76.97 | -4.11 | 0.63 | 1.67 | -3.89 | 1.66 | |
| | 300 | 4.75 | 0.85 | 0.97 | -79.17 | -4.23 | 0.12 | 1.68 | -3.92 | 1.66 | |

Table 2 — Mechanical constants of DyPn ($10^{10}$N/m$^2$)

| Material | Temp(K) | *E* | *B* | *G* | $C_p$ | *G/B* | $\sigma$ | $Z_A$ | *Ref.* |
|---|---|---|---|---|---|---|---|---|---|
| DyP | 0 | 4.05 | 2.63 | 1.63 | 0 | 0.62 | 0.25 | 0.82 | |
| | | | 8.54 | | | | | | [1] |
| | | 12.24 | 8.27 | 4.88 | | 0.59 | 0.25 | 0.64 | [2] |
| | 100 | 4.08 | 2.71 | 1.63 | -0.03 | 0.60 | 0.25 | 0.75 | |
| | 200 | 4.18 | 2.75 | 1.68 | -0.08 | 0.61 | 0.25 | 0.71 | |
| | 300 | 4.29 | 2.80 | 1.72 | -0.07 | 0.61 | 0.25 | 0.67 | |
| DyAs | 0 | 3.63 | 2.44 | 1.45 | 0 | 0.59 | 0.25 | 0.75 | |
| | | | 7.62 | | | | | | [1] |
| | 100 | 10.89 | 7.37 | 4.34 | | 0.59 | 0.25 | 0.63 | [2] |
| | | 3.75 | 2.50 | 1.50 | -0.07 | 0.60 | 0.25 | 0.69 | |
| | 200 | 3.85 | 2.55 | 1.54 | -0.08 | 0.60 | 0.25 | 0.65 | |
| | 300 | 3.96 | 2.59 | 1.59 | -0.13 | 0.61 | 0.25 | 0.62 | |
| DySb | 0 | 3.11 | 2.12 | 1.24 | 0 | 0.59 | 0.25 | 0.64 | |
| | | | 6.17 | 4.40 | | 0.71 | | 0.3 | [4] |
| | 100 | 3.22 | 2.17 | 1.28 | -0.04 | 0.59 | 0.25 | 0.59 | |
| | 200 | 3.31 | 2.21 | 1.32 | -0.4 | 0.60 | 0.25 | 0.56 | |
| | 300 | 3.40 | 2.26 | 1.36 | -0.12 | 0.60 | 0.25 | 0.53 | |
| DyBi | 0 | 2.94 | 2.01 | 1.17 | 0 | 0.58 | 0.25 | 0.61 | |
| | 100 | 3.04 | 2.06 | 1.21 | -0.03 | 0.59 | 0.25 | 0.56 | |
| | 200 | 3.13 | 2.11 | 1.25 | -0.08 | 0.59 | 0.25 | 0.53 | |

and atomic number. The elastic stiffness coefficient $C_{11}$ is increasing with temperature, which shows high inelasticity, is obtained for DyP at 300K. The hardness coefficient $C_{44}$ increases with temperature and is maximum at T=300K for DyP. The SOECs compared with literature[2] are deviating highly due to different method of calculations, negligence of interatomic interactions and negligence of van der Waal's forces. The nonlinear third order elastic constants $C_{111}$, $C_{112}$ and $C_{166}$ are of negative magnitude. $C_{123}$ shows maximum variation among third order elastic constants while $C_{456}$ remains invariable due to absence of vibrational energy. Cauchy formulation[25] under stress free condition $C_{123}^0 = C_{456}^0 = C_{144}^0$; $C_{12}^0 = C_{44}^0$; $C_{112}^0 = C_{166}^0$; are obeyed at 0K, which shows strong interaction between lattice ions with central force and each ion is situated at center of inversion. The Born stability formulation ($C_{11} + 2C_{12} > 0$, $C_{11} - C_{12} > 0$ and $C_{44} > 0$)[25] is fulfilled in present case for elastic stable selected DyPn. The mechanical parameters are calculated in the 0-300K temperature interval and the obtained results are placed in Table 2.

The Young modulus increases with temperature and decreases with mass number. Higher Young modulus represents higher stiffness by virtue of which DyP has highest and DyBi has lowest opposition against elastic deformation. Like Young, modulus the bulk and shear modulus are increasing with temperature and decreasing with atomic number. Higher bulk modulus indicates low compressibility while shear modulus indicates hardness of materials. Highest shear hardness is demonstrated at 300K by DyP whether lowest for DyBi at 0K. The resulting *G/B* values in present case are higher than 0.57, which shows chosen DyPn, are brittle[26]. The Cauchy pressure $C_p<0$, and $\sigma<0.3$ in present investigation reveals that DyP, DyAs, DySb and DyBi are brittle which validates earlier prediction of brittleness[24]. The Poison's ratio $\sigma$ =0.25 in Table 2 displays that interatomic forces are non-central and interatomic bondings are of ionic nature[24]. For isotropic cubic crystal $Z_A$=1, but in present case $Z_A \neq 1$which inference that chosen DyPn are of anisotropic in behaviour[25]. The values of direction dependent longitudinal velocities, shear velocities and thermal conductivities in temperature range 100-300K are presented in Table 3.

The ultrasonic velocity as a function of density and SOECs decreases from DyP to DyBi. The ultrasonic velocities are temperature dependent and increase with temperature. The most probable velocity i.e., Debye velocity measured from average of longitudinal and shear velocities are displayed in Fig. 1. The Debye velocity increases with temperature but decreases with atomic number. Maximum Debye velocity is for DyP at T=300K and in <111> direction while minimum for DyBi at T=100K in <100> direction. The computed Debye temperature is represented in Fig. 2. The Debye temperature is inverse function of molar mass and direct function of temperature, is highest for DyP at T=300K and lowest for DyBi at T=100K[25]. The curves in Fig. 2 are rising along <111> direction referring to higher Debye temperature. The thermal conductivity displayed in Table 2 is highest for DyP at T=100K along <111> direction as thermal conductivity is directly proportional to Debye temperature and is inversely related to temperature. Thus best thermal stability is obtained along <111> direction.

The calculated results of relaxation time and ultrasonic Grüneisen parameters (UGPs) along <100>, <110> and <111> directions and in the temperature range 100-300K temperature regime are placed in Table 4

Table 3 — Ultrasonic velocity, Debye average velocity ($10^3$m/s) and thermal conductivity ( in $10^2 Wm^{-1}K$) of DyPn

| Material | Temp(K) | Direction | $V_l$ | $V_{S1}$ | $V_{S2}$ | $\kappa$ |
|---|---|---|---|---|---|---|
| DyP | 100 | <100> | 7.74 | 4.06 | 4.06 | 1.66 |
| | | <110> | 7.39 | 4.06 | 4.68 | 1.30 |
| | | <111> | 7.26 | 4.48 | 4.48 | 2.05 |
| | 200 | <100> | 7.89 | 4.07 | 4.07 | 0.87 |
| | | <110> | 7.45 | 4.07 | 4.82 | 0.72 |
| | | <111> | 7.30 | 4.59 | 4.59 | 1.16 |
| | 300 | <100> | 8.04 | 4.08 | 4.08 | 0.61 |
| | | <110> | 7.52 | 4.08 | 4.97 | 0.53 |
| | | <111> | 7.34 | 4.69 | 4.69 | 0.88 |
| DyAs | 100 | <100> | 7.07 | 3.60 | 3.60 | 1.30 |
| | | <110> | 6.65 | 3.60 | 4.32 | 1.09 |
| | | <111> | 6.50 | 4.10 | 4.10 | 1.78 |
| | 200 | <100> | 7.21 | 3.61 | 3.61 | 0.69 |
| | | <110> | 6.72 | 3.61 | 4.46 | 0.61 |
| | | <111> | 6.54 | 4.20 | 4.20 | 1.02 |
| | 300 | <100> | 7.37 | 3.61 | 3.61 | 0.48 |
| | | <110> | 6.79 | 3.61 | 4.61 | 0.44 |
| | | <111> | 6.59 | 4.30 | 4.30 | 0.77 |
| DySb | 100 | <100> | 6.62 | 3.18 | 3.18 | 0.93 |
| | | <110> | 6.07 | 3.18 | 4.12 | 0.86 |
| | | <111> | 5.88 | 3.84 | 3.84 | 1.52 |
| | 200 | <100> | 6.76 | 3.19 | 3.19 | 0.49 |
| | | <110> | 6.14 | 3.19 | 4.27 | 0.47 |
| | | <111> | 5.92 | 3.94 | 3.94 | 0.87 |
| | 300 | <100> | 6.92 | 3.19 | 3.19 | 0.34 |
| | | <110> | 6.21 | 3.19 | 4.40 | 0.35 |
| | | <111> | 5.96 | 4.04 | 4.04 | 0.66 |
| DyBi | 100 | <100> | 5.83 | 2.75 | 2.75 | 0.74 |
| | | <110> | 5.31 | 2.75 | 3.66 | 0.71 |
| | | <111> | 5.12 | 3.38 | 3.38 | 1.29 |
| | 200 | <100> | 5.97 | 2.75 | 2.75 | 0.39 |
| | | <110> | 5.37 | 2.75 | 3.79 | 0.39 |
| | | <111> | 5.16 | 3.47 | 3.48 | 0.74 |
| | 300 | <100> | 6.10 | 2.76 | 2.76 | 0.27 |
| | | <110> | 5.44 | 2.76 | 3.91 | 0.28 |

The time duration to achieve original condition of deformed phonons due to thermal agitation is termed as relaxation time. The time involves establishing thermal equilibrium is of the order $10^{-11}$s, which shows that selected DyPn possess semi-metallic in nature. A dimensionless quantity the Grüneisen parameter introduces a change in vibrational frequency due to change in volume of lattice under pressure. The Grüneisen parameter $\langle \gamma_i^j \rangle$, where '*i*' refers for mode and '*j*' refers for direction of propagation, is an interlinking variable between bulk modulus, thermal expansion coefficient and specific heat is evaluated by the formulae based on second- and third order elastic constants for longitudinal and shear modes in <100>,

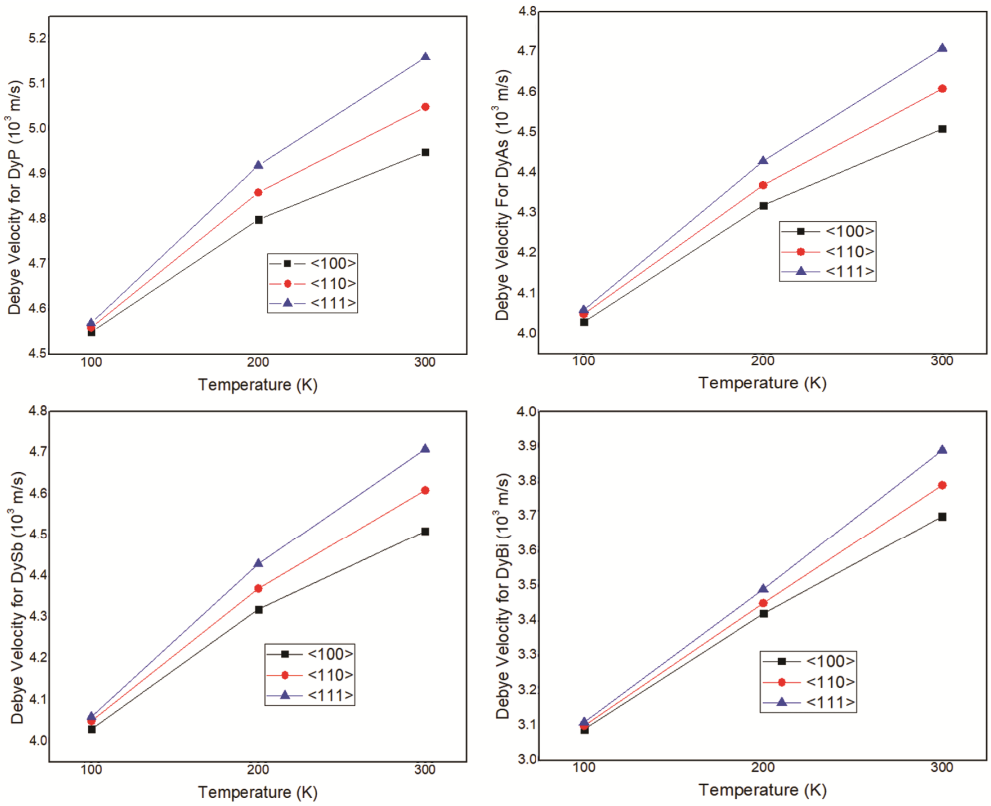


Fig. 1 — The Debye velocity along ($10^3$ m/s) in <100>, <110> and <111> directions for DyPn

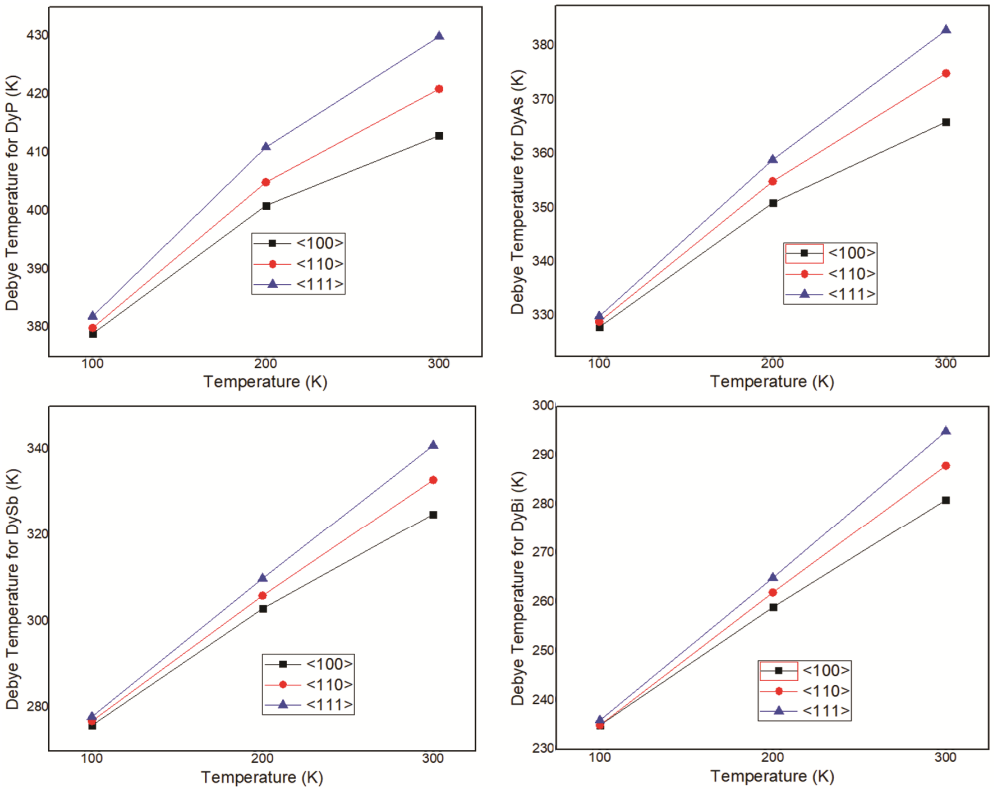


Fig. 2 — The Debye temperature (K) along <100>,<110> and <111> directions for DyPn

Table 4 — The relaxation time ($10^{-11}$s), average and Gruneisen parameters for DyPn

| Material | Temp(K) | Direction | $\tau_{th}$ | $<\gamma_i^j>$ | $<\gamma^2>_l$ | $<\gamma^2>_{S1}$ | $<\gamma^2>_{S2}$ |
|---|---|---|---|---|---|---|---|
| DyP | 100 | <100> | 17.98 | 0.5271 | 2.1805 | 0.1492 | 0.1492 |
| | | <110> | 13.45 | 0.8742 | 3.2684 | 0.2969 | 3.4862 |
| | | <111> | 20.59 | 0.7211 | 2.2655 | 2.1165 | 2.1165 |
| | 200 | <100> | 5.97 | 0.5146 | 2.0914 | 0.1464 | 0.1464 |
| | | <110> | 4.43 | 0.8440 | 3.0638 | 0.2632 | 3.3556 |
| | | <111> | 6.75 | 0.6998 | 2.1261 | 2.0384 | 2.0384 |
| | 300 | <100> | 3.80 | 0.5028 | 2.0105 | 0.1437 | 0.1437 |
| | | <110> | 2.88 | 0.8154 | 2.8836 | 0.2350 | 3.2320 |
| | | <111> | 4.36 | 0.6800 | 2.0011 | 1.9651 | 1.9651 |
| DyAs | 100 | <100> | 15.67 | 0.528 | 2.25 | 0.1466 | 0.1466 |
| | | <110> | 12.08 | 0.871 | 3.2977 | 0.2506 | 3.6452 |
| | | <111> | 19.12 | 0.7264 | 2.2998 | 2.2145 | 2.2145 |
| | 200 | <100> | 5.69 | 0.5147 | 2.1565 | 0.1438 | 0.1438 |
| | | <110> | 4.44 | 0.8392 | 3.0904 | 0.2234 | 3.5016 |
| | | <111> | 6.82 | 0.7042 | 2.1539 | 2.1289 | 2.1289 |
| | 300 | <100> | 3.71 | 0.5027 | 2.0734 | 0.1412 | 0.1412 |
| | | <110> | 2.91 | 0.8101 | 2.913 | 0.2015 | 3.3715 |
| | | <111> | 4.51 | 0.6840 | 2.0266 | 2.0518 | 2.0518 |
| DySb | 100 | <100> | 12.47 | 0.5287 | 2.3874 | 0.1426 | 0.1426 |
| | | <110> | 10.15 | 0.8641 | 3.3804 | 0.1920 | 3.9404 |
| | | <111> | 16.78 | 0.7364 | 2.3712 | 2.3965 | 2.3965 |
| | 200 | <100> | 5.00 | 0.5151 | 2.2879 | 0.1401 | 0.1401 |
| | | <110> | 4.04 | 0.8315 | 3.1765 | 0.1745 | 3.7849 |
| | | <111> | 6.47 | 0.7134 | 2.2192 | 2.3041 | 2.3041 |
| | 300 | <100> | 3.29 | 0.5028 | 2.2020 | 0.1378 | 0.1378 |
| | | <110> | 2.70 | 0.8019 | 3.0049 | 0.1604 | 3.6475 |
| | | <111> | 4.33 | 0.6926 | 2.0883 | 2.2229 | 2.2229 |
| DyBi | 100 | <100> | 12.15 | 0.5294 | 2.4415 | 0.1416 | 0.1416 |
| | | <110> | 9.99 | 0.8627 | 3.4238 | 0.1779 | 4.055 |
| | | <111> | 16.16 | 0.7407 | 2.4031 | 2.467 | 2.467 |
| | 200 | <100> | 5.20 | 0.5155 | 2.3398 | 0.1392 | 0.1392 |
| | | <110> | 4.26 | 0.8295 | 3.22 | 0.1626 | 3.8947 |
| | | <111> | 6.79 | 0.7172 | 2.2481 | 2.3718 | 2.3718 |
| | 300 | <100> | 3.47 | 0.5030 | 2.2527 | 0.1370 | 0.1370 |
| | | <110> | 2.90 | 0.7996 | 3.0496 | 0.1502 | 3.7550 |
| | | <111> | 4.66 | 0.6962 | 2.1155 | 2.2892 | 2.2892 |

<110> and <111>[22]. The Grüneisen parameter being function of second-, and third-order elastic constants is dependent on temperature and decreases with temperature. The highest average Grüneisen constant is found along <110> at T=100K for DyP and decreases with mass number. The squared average of Grüneisen constant is found largest for shear mode along <110> direction while longitudinal mode dominates in <100> and <111> directions and follow the order DyP>DyAs>DySb>DyBi. For linear restoring forces, the frequency of phonon is independent of volume by virtue of which, thermal expansion coefficient vanishes and in turn $\gamma = 0$. In present case $\gamma \neq 0$ which inference that restoring forces are non-linear. The results obtained for average Grüneisen parameter and average squared Grüneisen parameter are compared with other B1 structured pnictides[12-16] to validate theory due to unavailability of similar literatures. The obtained results will provide base for further studies and researches.

## 4 Conclusion

The elastic constants are evaluated for DyPn (Pn = P, As, Sb and Bi) and are validated successfully applying Born-Mayer interaction theory. The DyPn are found to be elastic and mechanically stable under

stress free condition. The brittle nature of DyPn is predicted by the hardness to fracture ratio greater than 0.57. The Debye velocity increases with temperature but decreases with mass number. Maximum Debye velocity is for DyP at T=300K and in <111> direction while minimum for DyBi at T=100K in <100> direction. The Debye temperatures and thermal conductivities are found to be highest along <111> direction. The average Grüneisen constant is found to be highest along <110> at T=100K for DyP and decreases with mass number.

**Acknowledgement**

The authors gratefully acknowledge the financial support received from the Department of Science & Technology, New Delhi and Council of Science & Technology, U.P.

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